MASS SPECTROMETER FOR IECM

Part I - Description

R. C. Ruff
ES74
Marshall Space Flight Center
Huntsville, Alabama 35812

D. R. Taeusch
Space Physics Research Laboratory
University of Michigan
Ann Arbor, Michigan 48105

Part II - Measurement Concepts

W. A. Oran and T. Rathz
ES72/ES74
Marshall Space Flight Center
Huntsville, Alabama 35812

BACKGROUND

The Induced Environment Contamination Monitor (IECM) is to be flown on the first six Shuttle Orbital Flight Tests as Development Flight Instrumentation. The Mass Spectrometer (MS) is incorporated into the IECM to perform molecular column density and molecular return flux measurements as specified by the Shuttle Transportation System--Payload Contamination Requirements Definition Group[1] (CRDG).

The purpose of the MS measurements is two-fold. The first is to define what emitted molecules are being backscattered to the Shuttle bay for correlation with deposition type measurements being made by other IECM instruments. The second is to define the column density of the gas cloud (induced atmosphere) through which optical experiments must look. The sources of this emitted gas are from leaks, vents, thruster firings, and off-gassing and out-gassing of surfaces. These gases, as they flow away from the spacecraft at thermal speeds, collide with the ambient atmosphere molecules which have a relative velocity of 8 km/sec with respect to the spacecraft. This collision process causes a small fraction of the emitted gas to be deflected back into the 0.1 steradian collimated view of the MS. The MS will count all molecules from 2 to 150 atomic mass units (amu) which it sees. Interpretation of these counts depends on how much is known about the scattering process. A gas release calibration experiment to quantify the scattering process will be incorporated into the MS.

In Part I of this paper is presented a description of the MS and a discussion of its measurement capabilities. In Part II is presented a conceptual simulation of the in situ measurements and a discussion of how the expected backscattering is related to the column density and the kinematics of the scattering process. This is done to help define the relationship between the measurements and actual column density so that preferred vehicle maneuvers and attitudes can be established which will optimize the scientific results.

PART I

1.0 Introduction

The MS system, consisting of a quadrupole mass analyzer and its associated electronics, is similar to several which flew on Atmospheric Explorer satellites.[2] The basic modifications for the IECM application are the additions of an inlet collimator, a gas source calibration system, and a resealable valve mechanism. The MS system is being developed and built by the University of Michigan, Space Physics Research Laboratories. Two identical units will be delivered to Marshall Space Flight Center, Space Sciences Laboratory, for integration and operation aboard Shuttle. A photograph of unit 1 is shown in Figure 1.

2.0 Description of Instrument

The MS system is mounted in the IECM such that the center line of the conical view is perpendicular to the top of the IECM which is mounted parallel to the Shuttle bay floor. Therefore, the view is perpendicular to the long (X) axis of the Shuttle, parallel to the Z axis. The sequential operations of the MS are all controlled by the data system of the IECM. The specific subsystems of the MS are described below.

2.1 Mass Sensor Subsystem

The mass sensor consists of a thermalizing chamber and electron impact ionization source, a hyperbolic-rod quadrupole analyzer, and an off-axis electron multiplier. The quadrupole analyzer is tuned for flat top peaks and measurements are made by digitally stepping from peak to peak.
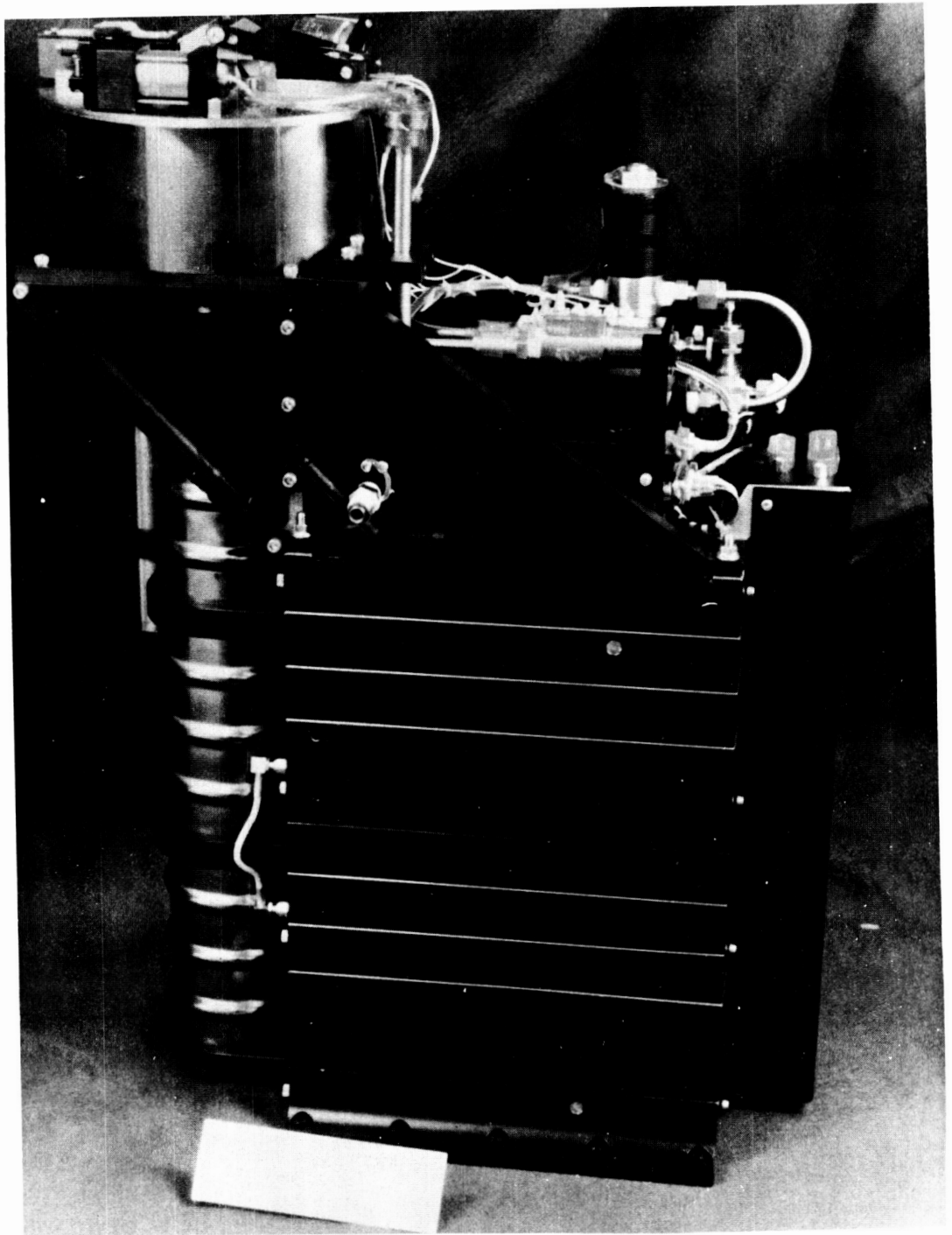
Figure 1. Mass Spectrometer for
IECM, Unit 1

The MS is capable of monitoring molecules with a mass to charge ratio from 2 to 150 with a resolution such that contributions from adjacent mass peaks are less than one part in 10^3. The electron multiplier has 14 stages of electron multiplication. This provides a current pulse of approximately 10^6 electrons per ion to a pulse counting circuit. The pulse amplifier is limited to a maximum counting rate of 5×10^7 pulses/sec. The sensor subsystem has an overall sensitivity of 10^{-5} amps/torr which implies an internal number density of 500 molecules/cm^3 for every count/sec.

2.2 Data and Control Subsystem

The amplified pulses from the electrometer are supplied to a 24 bit accumulator (16,777,215 counts). A floating point converter compresses the data from 24 bits to 13 bits consisting of 9 bits of linear number and 4 bits of multiplier or decimal position. The 9 bits equal 512 counts, which give a digital resolution of 0.2% to 0.4% for all counts above 512.

Since the IECM data system is an 8 bit system, two 8 bit words will be given to the IECM processor every 2 seconds during slow sweep and every 200 MS during fast sweep. One of the 3 bits not used for counts will be used to "mark" the start of a sweep. Since the mass sweep starts at mass zero and indexes one mass each time the IECM accepts the 16 bits, no further data is required for automatic reduction of the measured mass.

The remaining 2 bits will be used to multiplex digitized analog housekeeping words. Four masses will be required to assemble one 8 bit housekeeping word. Thus, it is possible to have 38, 8 bit words during one scan of 150 masses.

Several functions of the MS are initiated and timed by the IECM control system. The IECM interrogates the MS for the two 8 bit data words. The intervals between interrogation control the integration time for accumulating counts. It is presently planned that the IECM would have two preset interrogation rates--a slow scan with 2 second integration and a fast scan with 0.2 second integration at each amu (atomic mass unit) peak.

The IECM has three additional controls over the MS. A "Gas Calibration" signal initiates release of an isotopically labeled gas mixture. A "Special Mass" signal requests an abbreviated sweep from 2 to 48 amu. The "Valve Close" signal triggers a mechanism to seal the orifice of the MS before re-entry.

Figure 2 is a pictorial description of the abbreviated sweep and the normal sweep which alternates between sweeping from 2 to 150 amu and 150 integrations of the water peak at 18 amu. Both the normal sweep and the abbreviated "Special Mass" sweep take 8 steps across amu 28 to act as a check on the operation of the instrument.

FIGURE 2. PICTORIAL DESCRIPTION OF NORMAL AND ABBREVIATED MASS SWEEPS
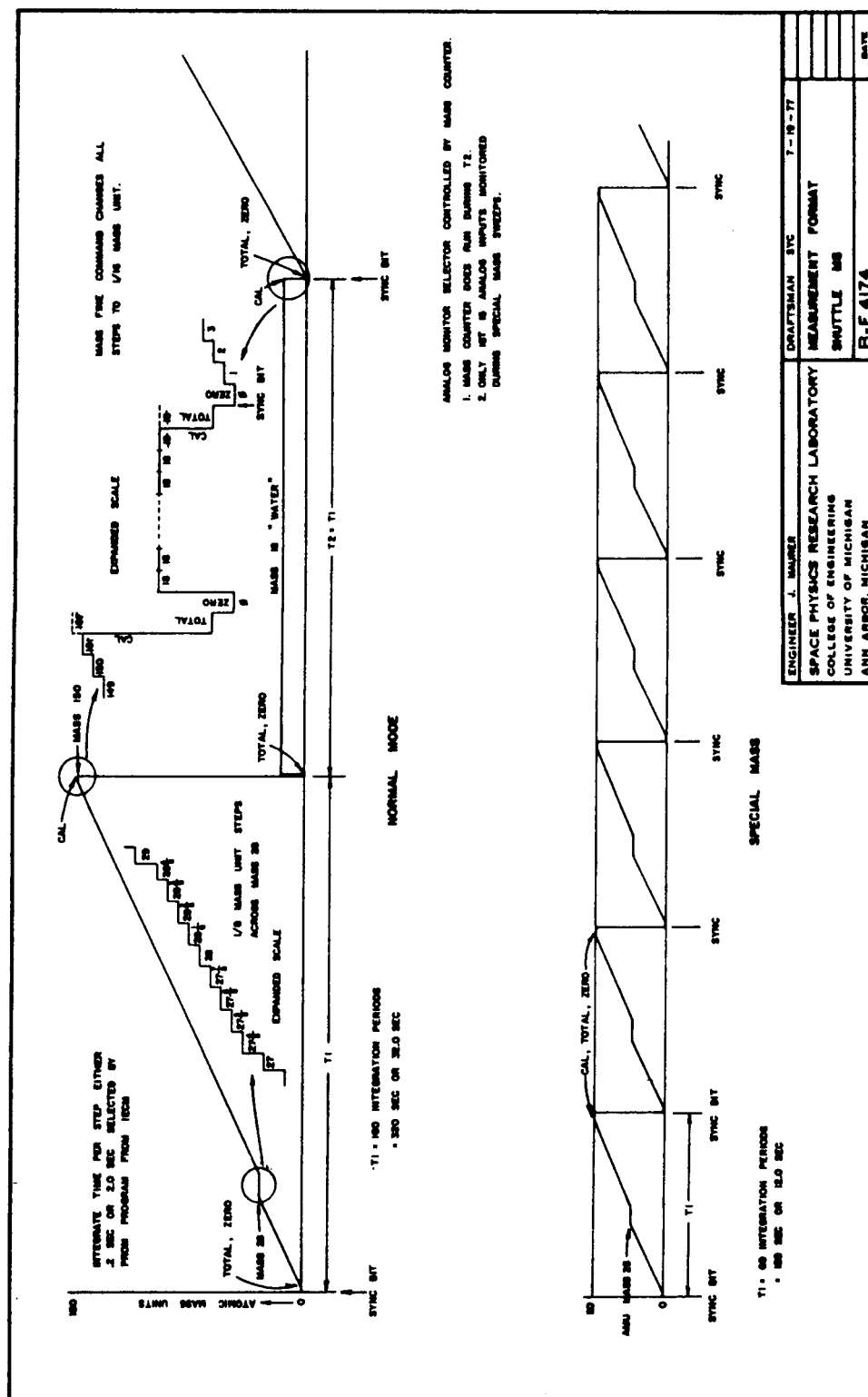
2.3 Collimator Subsystem

The collimator design consists of three chevron baffles plus an orifice (Figure 3) which separates the flow such that those molecules which enter the orifice at an angle greater than 10° from the normal to the orifice are directed into a chamber which contains a number of sintered zirconium powder "getter" pumps. The theoretical curve of normalized ion source response to angle of incidence of the flow field is given in Figure 4.

The size and amount of getter material required depends on the gas load for which it is designed. This should be minimized. However, the orifice must be large enough to allow an adequately short vacuum time constant for the internal gas. It was decided that a 3 mm diameter orifice was as small as seemed engineeringly feasible, gave an adequately short time constant, and gave a low enough gas load to be handled by a reasonable number of getters.

The conductance of a 3 mm diameter knife edge orifice is 850 cm^3/sec. The ion source volume to which the vacuum time constant applies is that volume behind the last chevron baffle in front of the quadrupole tube. The collimator volume itself is, of course, pumped by the getters and the volume of the quadrupole analyzer is pumped by a separate appendage pump. The conductance from the ion source to the analyzer section is estimated to be 70 cm^3/sec which is small compared to the inlet orifice

ORIFICE

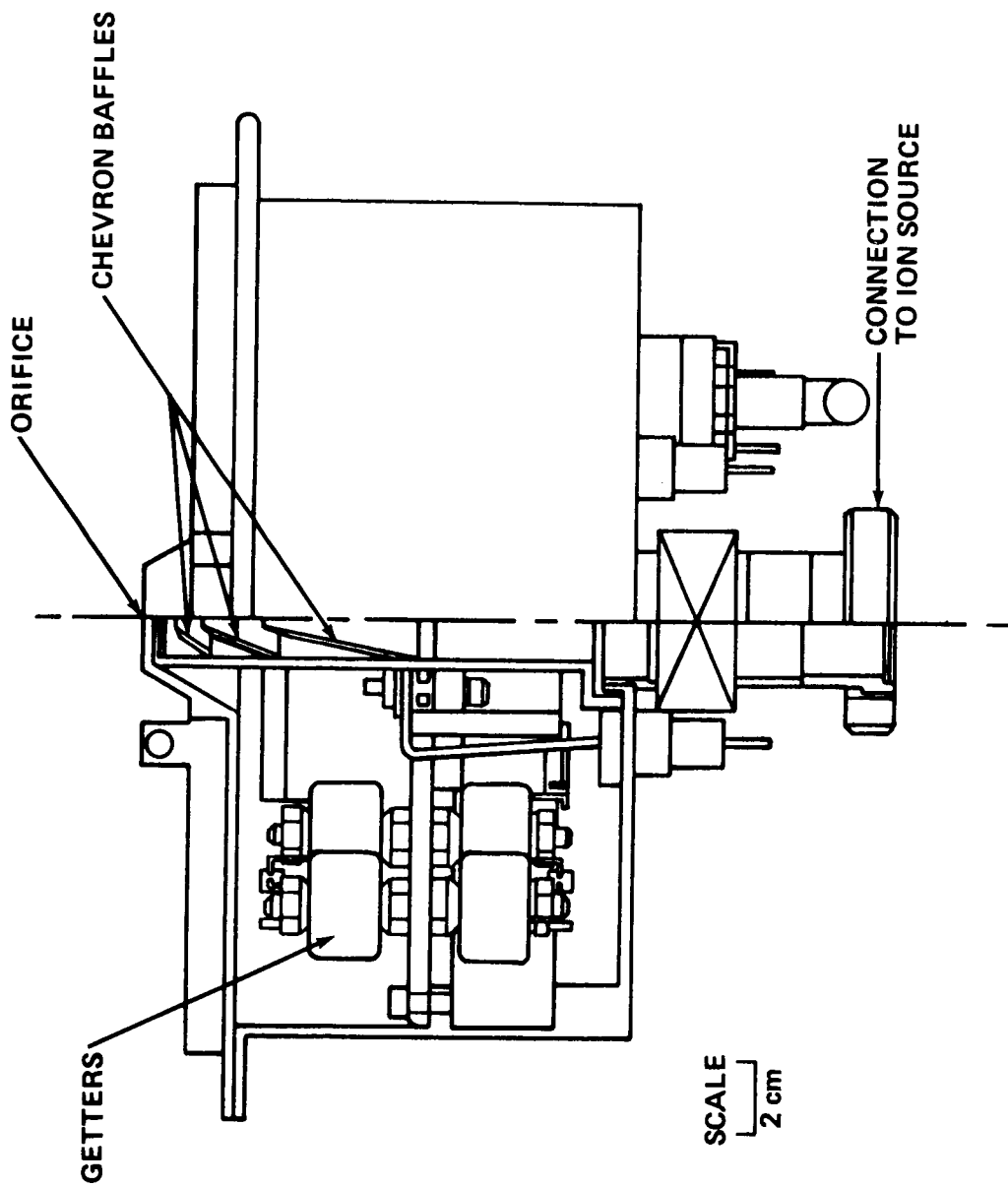CHEVRON BAFFLES

GETTERS

CONNECTION
TO ION SOURCE

SCALE
2 cm

FIGURE 3. COLLIMATOR DESIGN

$$R = \frac{2}{\pi} \left\{ \cos^{-1}\left(\frac{a}{2r_o}\right) - \frac{a}{2r_o}\left[1 - \left(\frac{a}{2r_o}\right)^2\right]^{\frac{1}{2}}\right\}$$

$a = \ell \; TAN \; \alpha$

$\ell = 1.7mm$ = SEPERATION OF ORIFICES

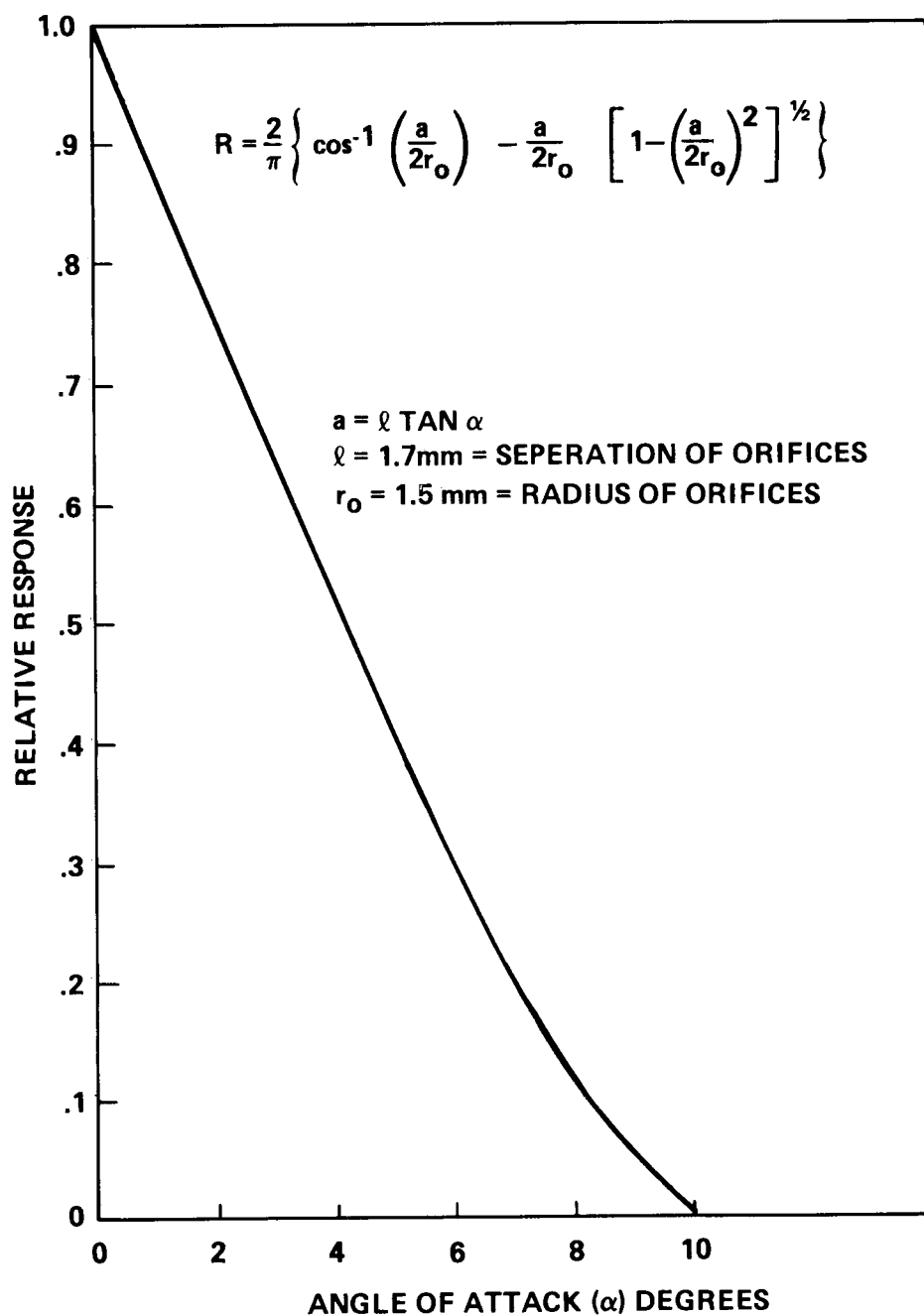$r_o = 1.5 \; mm$ = RADIUS OF ORIFICES

FIGURE 4. NORMALIZED ION SOURCE RESPONSE TO ANGLE OF INCIDENCE OF GAS FLOW

conductance. Therefore, the ion source density will respond primarily to the external changes in inlet flux. The ion source volume is a cylinder about 1 cm in radius and about 10 cm long, or about 31 cm^3. This gives a vacuum time constant for the volume of about 3.6×10^{-2} seconds, which is believed more than adequate for the intended use.

The maximum gas load on the collimator will be when the normal to the orifice is pointed directly into the velocity vector during orbit at 250 km altitude. This gas load is expected to be 2×10^{15} part/cm^2 sec. The orifice area is 7×10^{-2} cm^2; therefore, the gas load will be 1.41×10^{14} part/sec or 4.4×10^{-3} $\frac{torr\ cm^3}{sec}$ at a collimator temperature of 300°K. It is expected that the maximum time this flux would be encountered during a Shuttle mission would be 100 hrs.; therefore, the maximum loading of the getters would be about 1600 torr cm^3 per mission. It was decided to incorporate sufficient getters to provide a pumping speed of 5 times the incoming gas load.

2.4 <u>Inlet Valve Mechanism</u>

In the past mass spectrometers which flew on orbital satellites were able to use simple one-time break-off tubes as the valve mechanism. However, since the MS is expected to fly on at least six OFT

missions, a mechanism was developed for resealing the orifice before re-entry to protect the getters, ion source, and electron multiplier from contamination.

The valve mechanism developed to meet the various mechanical and thermal requirements is shown in Figure 1. The valve for prelaunch sealing (called opening valve) must be bakeable to 350°C and must, therefore, utilize a metal sealing ring under high compression. This force is generated by a ceramic rod in compression. At the appropriate time after orbit is achieved, a solenoid is activated which releases a spring loaded arm. The momentum of this arm is used to break the ceramic rod. The metal cap holding the metal sealing ring is then released and swings away in a 180 degree arc to expose the mass spectrometer orifice to space. The closing valve does not need to be exposed to the 350°C bake and, therefore, utilizes a rubber 0-ring with much less compression force. Upon receipt of the proper signal from the IECM, a solenoid is again used to release the spring loaded arm which swings the 0-ring against the orifice.

It is expected that unless a large amount of contamination is enountered, the mass spectrometer will need minimal refurbishment between flights. This would consist of resealing the metal opening valve while under a nitrogen purge and then a simple bake to remove the large nitrogen gas load from the getters. The sealing mechanism used for this and all other vacuum bake operations is a copper pinch-off tube.

A major contamination of the instrument such as a valve malfunction or high pressure during a Shuttle bay door closing test would require a major refurbishment which involves cleaning or replacement of the electron multiplier or actual dismantling of the quadrupole for cleaning.

2.5 Gas Source Calibration

In order to better relate the measured ion-source densities in the mass spectrometer on the IECM to the effluent densities and resulting column densities of contaminant gases, an inflight calibration will be performed. The calibration will consist of activation of a gas release system which will emit a known flux of isotopically labeled water and neon into the collimated view of the MS, and the backscattered flux will be monitored. A sufficient quantity of the calibration gas mixture will be provided to enable a 45-minute calibration, during which time the angle of attack of the mass spectrometer pointing vector will be varied between 0 and 180°. The relationship between the backscattered flux and the known effluent flux density as a function of angle of attack will thus be obtained. This will provide the calibration needed to interpret the measurements of Shuttle effluents. Moreover, these calibration measurements provide the basis for evaluating the differential scattering cross sections for 8 km/s collisions, a measurement of basic physical importance.

The calibration source will utilize a 350 cm^3 vessel pressurized to 10 atmospheres of ^{22}Ne, with deuterated liquid water (D_2O) in sufficient quantity to maintain its vapor pressure (23.5 torr @ 25°C). A total flux

of 3×10^{19} cm^{-2}s^{-1} is maintained by regulating the pressure to 4.5 lb/in^2 and restricting the flow to 1000 torr cm^3/s to a capillary array of 1 cm^2 cross sectional exit area. A block diagram of the system is shown in Figure 5. The capillary array collimates the effluent to about a 10° half angle stream into the collimated view of the MS. Under these conditions the water flow rate would start at about 4 torr cm^3/s, increase to 100 torr cm^3/s at 45 minutes after initiation, and then drop to 30 torr cm^3/s when the Ne was depleted, if maintained at 25°C. This is shown in Figure 6.

The ^{22}Ne and D$_2$O gases were selected for several reasons. Since water is such a large component of the Shuttle effluent and since water is a major contaminant for many infrared observations, D$_2$O was chosen to elucidate the role of water in the ambient and self-scattering mechanisms while not actually being masked by natural H$_2$O contamination. Neon was chosen to provide a comparison scattering mechanism for a monoatomic gas near the same mass. These two gases should allow a determination of the scattering cross section as related to inelastic and elastic collisions. Later OFT flights probably will utilize H$_2$^{18}O in place of D$_2$O to further study the inelastic scattering mechanism.

3.0 Operational Characteristics

Once the MS has been turned on in orbit and the orifice valve has been opened, the MS will automatically step through its preprogrammed sequence of mass peaks and provide the data to the IECM. It is presently planned to have three modes of operation for the MS.
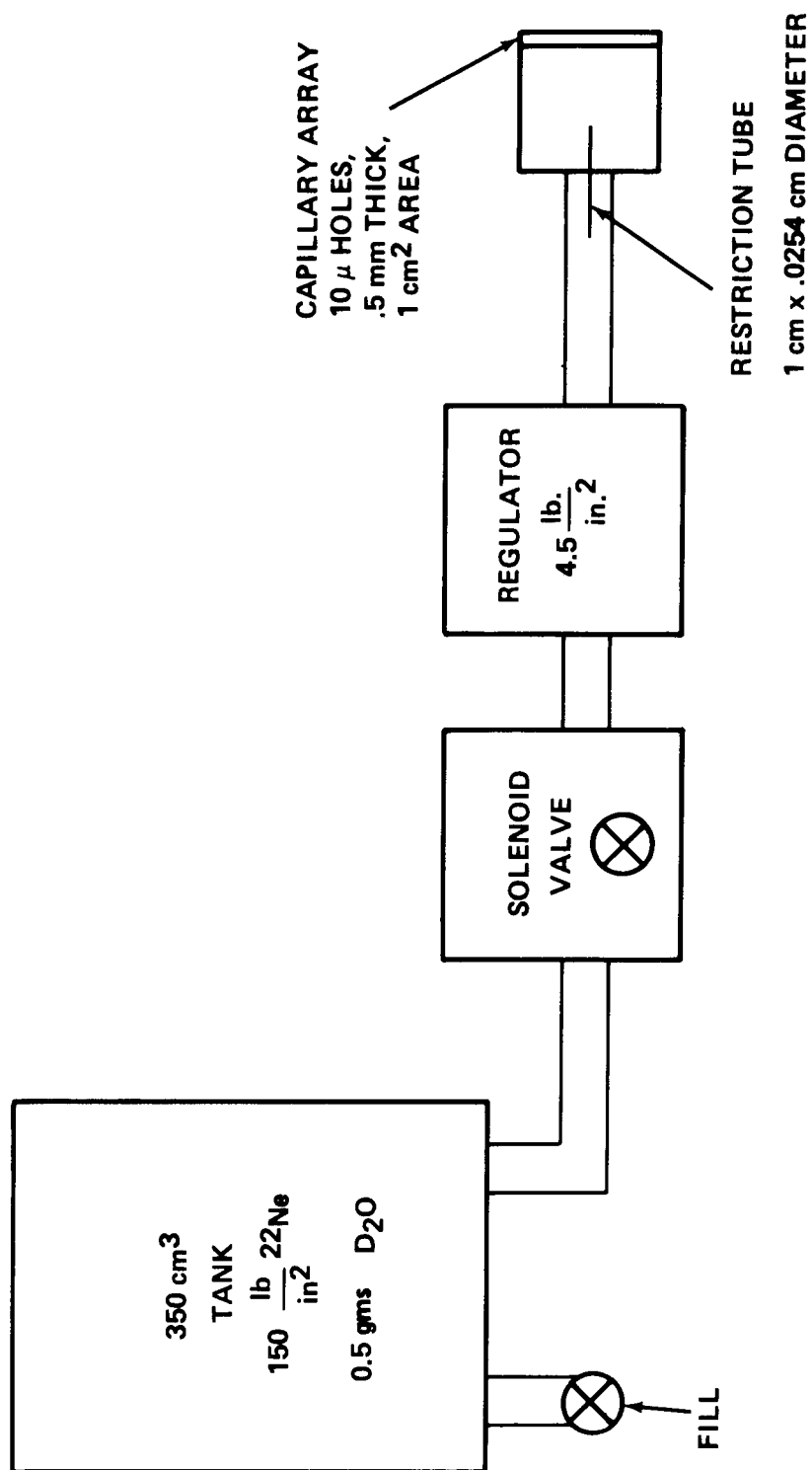
CAPILLARY ARRAY
10 μ HOLES,
.5 mm THICK,
1 cm^2 AREA

RESTRICTION TUBE
1 cm x .0254 cm DIAMETER

REGULATOR
4.5 $\frac{lb.}{in.^2}$

SOLENOID
VALVE

350 cm^3
TANK
150 $\frac{lb}{in^2}$ ^{22}Ne
0.5 gms D$_2$O

FILL

FIGURE 5. BLOCK DIAGRAM OF GAS RELEASE SYSTEM
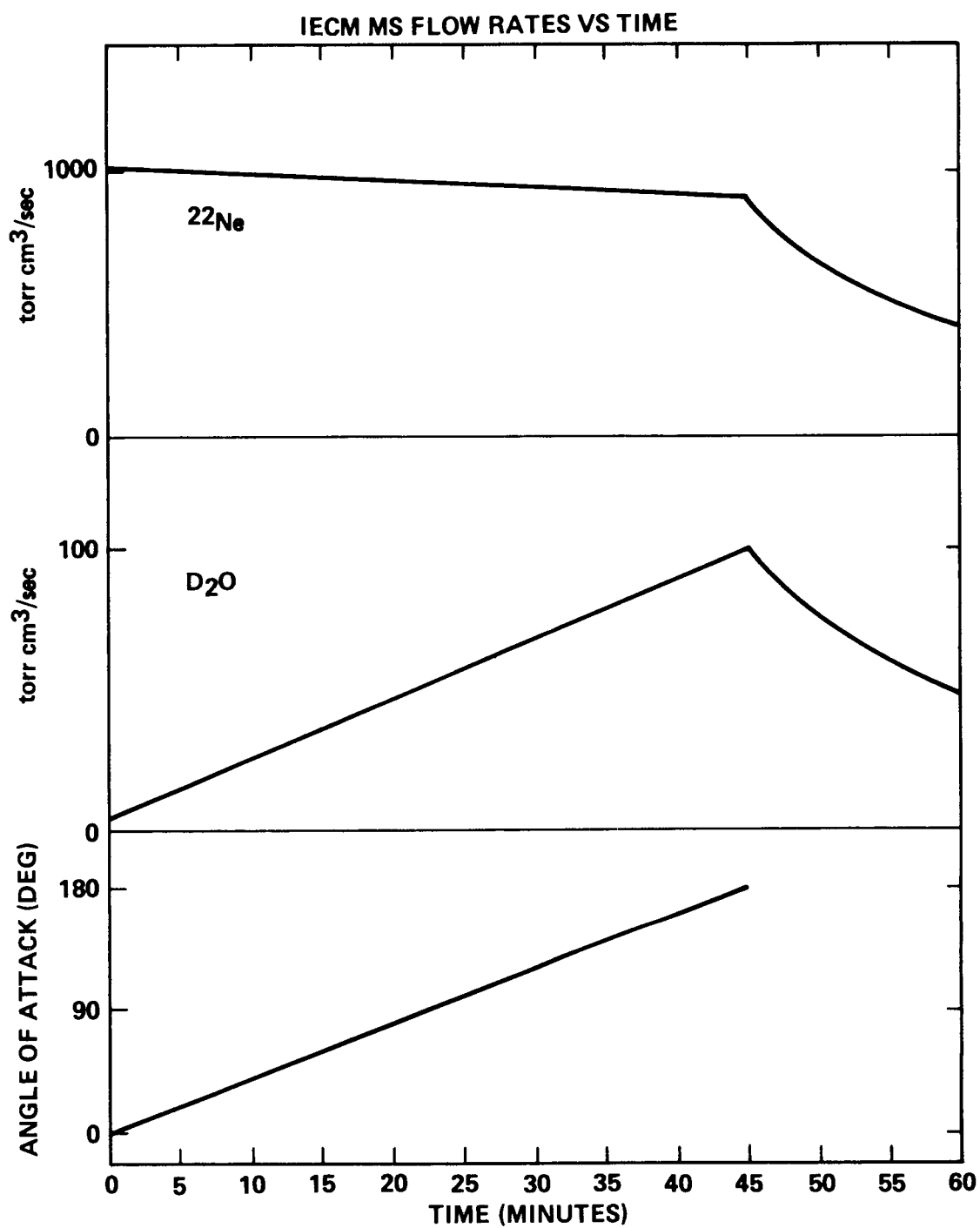
IECM MS FLOW RATES VS TIME

FIGURE 6. GAS RELEASE FLOW RATE AS A FUNCTION OF TIME

The normal mode will be for the IECM to interrogate the MS only once every two seconds. As described earlier, the MS would step through a complete sweep from 2 to 150 amu and then alternate with 150 measurements of the water peak (amu 18) before repeating. This mode provides a relatively long integration time for those masses with very low partial pressures while also measuring temporal fluctuations of the important contaminant, water. It does, however, limit data on masses other than water to once every 10 minutes.

The fast sweep mode is simply generated by the IECM speeding up its interrogation rate to once every 0.2 seconds. The alternating sweep with amu 18 is still in operation. However, each mass is now recorded once every 1.0 minute. This mode is principally planned for the Remote Manipulator operation where the IECM is picked up and moved around over various surfaces of the Shuttle.

The special mass mode is an abbreviated sweep mode. It can be activated at any time by a signal from the IECM. In this mode the MS only sweeps over the range from 2 to 48 amu. This mode was incorporated to provide a better time resolution during the gas calibration sequence. This mode can, however, be used at any time desired with either the normal or fast sweep mode.

4.0 Measurement Capabilities vs. Requirements

The measurement capabilities need to be analyzed at the two extremes of flow rate.

The flow regimes of interest are of two basic kinds, one being the directed stream flow superimposed on a Maxwell-Boltzmann distribution of thermal speeds which is due to the spacecraft vehicle velocity with respect to a stationary ambient atmosphere. This flow is of importance only at small angles of attack, i.e., small angles between the normal to the inlet orifice and the directed stream direction. The other flow of interest is that due to the scattered molecules which are the result of emitted spacecraft gas which collides with the free stream molecules and causes a small fraction of them and the ambient gas to be returned to the mass spectrometer inlet. This flow may be detectable at all angles of attack, and can be determined at small angles of attack as long as the molecule being looked at has a mass different from the ambient stream gas.

4.1 Directed Stream Flow

For a flux of known quantity through the inlet orifice we wish to know the flux which successfully passes through the collimator into the ion source region.

Calculations have been made to relate the angular spread of ambient gas velocities due to their thermal velocities superimposed on the flow velocity generated by the Shuttle velocity. The results are shown in Figure 7. The different s values were chosen in the range of expected ambient gas molecules and expected temperature range. It can be seen that the ambient gas molecules can reach the ion source at angles greater than 10 degrees to the velocity vector.
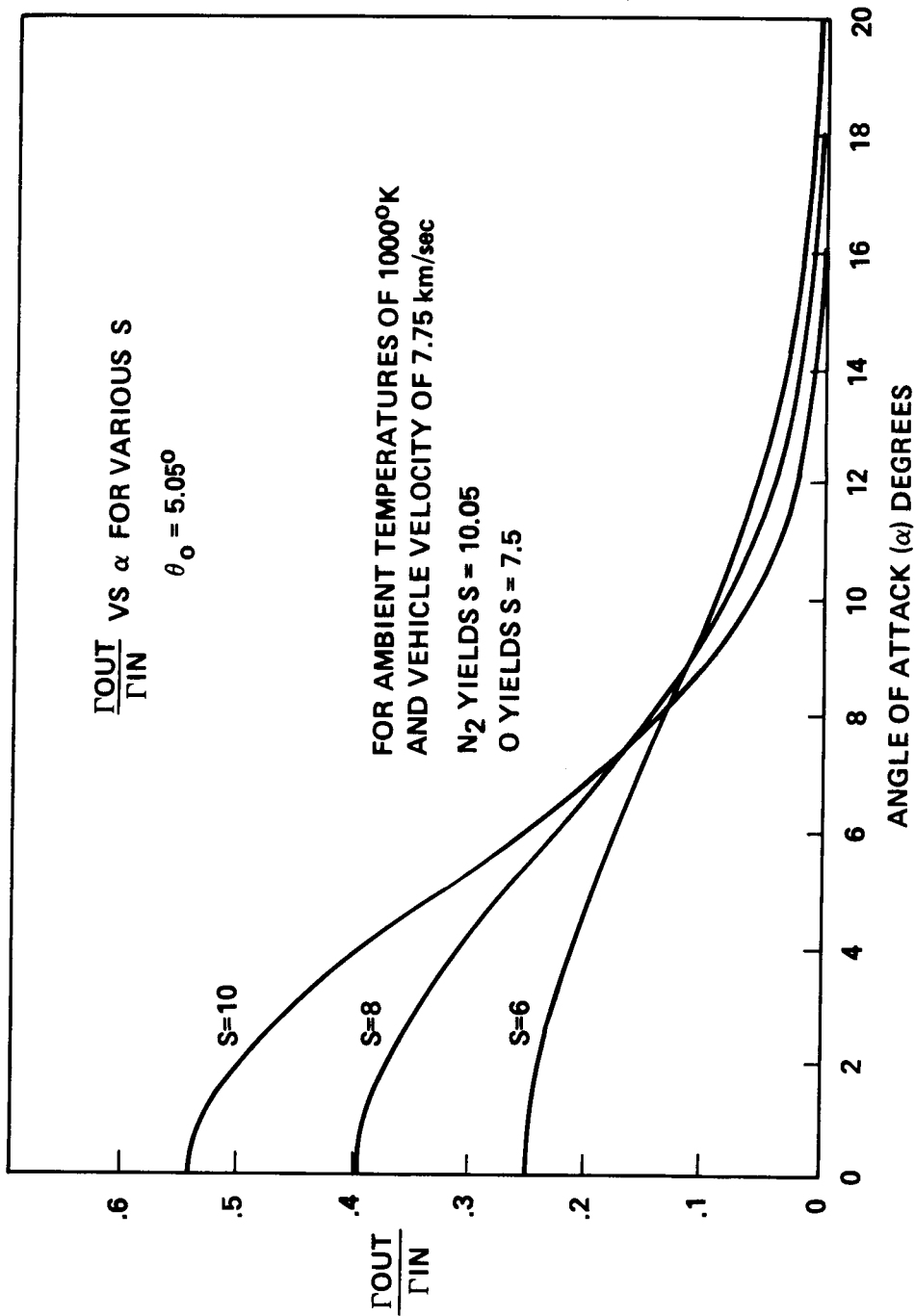
FIGURE 7.   RATIO OF FLUX THROUGH INLET ORIFICE, Γ IN, TO FLUX WHICH REACHES ION SOURCE Γ OUT.

The plot shows $\frac{\Gamma \text{OUT}}{\Gamma \text{IN}}$ VS α FOR VARIOUS S

$\theta_o = 5.05^o$

FOR AMBIENT TEMPERATURES OF 1000^oK AND VEHICLE VELOCITY OF 7.75 km/sec

N_2 YIELDS S = 10.05

O YIELDS S = 7.5

ANGLE OF ATTACK (α) DEGREES

$\frac{\Gamma \text{OUT}}{\Gamma \text{IN}}$

Curves labeled S=10, S=8, S=6

Using the appropriate Jacchia[3] values for density times stream velocity at 250 km altitude at zero angle of attack:

O_2	yields	1×10^{14} part/cm^2 sec
N_2	yields	7×10^{14} part/cm^2 sec
O	yields	1.2×10^{15} part/cm^2 sec

We get densities N_i in the ion source of

$$N_i (O_2) \text{ due to } O = 1.98 \times 10^{10} \text{ part/}cm^3$$

$$N_i (O_2) \text{ due to } O_2 = 5.34 \times 10^9 \text{ part/}cm^3$$

or $\quad N_i (O_2)$ total $= 2.51 \times 10^{10}$ part/cm^3

and $\quad N_i (N_2) \qquad\quad = 3.22 \times 10^{10}$ part/cm^3

Recalling that the MS has a sensitivity of 1 count/sec for every 500 part/cm^3, we have the MS measurement rate N of

$$N (O_2) = 5.02 \times 10^7 \text{ counts/sec}$$

$$N (N_2) = 6.44 \times 10^7 \text{ counts/sec}$$

This rate is near the maximum rate for the pulse counting amplifier and above the maximum accumulator count for a 2-second integration. However, these numbers result only when the MS is looking directly at the ambient gas. Several degrees off this angle will drop the rate to a manageable value.

4.2 Random Flux

In the case of random fluxes of effluent gases being backscattered to the MS, we must determine the minimum detectable flux rate. The

requirement of the CRDG is to be able to measure a random flux of 10^9 $cm^{-2}sec^{-1}sr^{-1}$. Assuming this flux to be water, we get a density in the ion source of

$$N_i (H_2O) = 2.86 \times 10^3 \ part/cm^3.$$

The MS sensitivity reduces this to

$$N (H_2O) = 5.71 \ counts/sec$$

which has a statistical uncertainty of 2.5 counts/sec.

Although this accuracy is low, it should be remembered that the data analysis can reduce the uncertainty by combining several successive sweeps to increase the sensitivity. Also, the normal data rate is for a two-second integration period.

5.0   Data Reduction

As has been shown in the previous section, the counting ratio will vary geratly depending on a variety of Shuttle operations and atmospheric conditions. For this reason, a large part of the past mission data reduction will consist of correlating MS measurements to the Shuttle maneuvers and attitude. Another important correlation will be to the Shuttle altitude to determine the ambient gas particle density. Using these correlations and an estimate of scattering cross sections, it is planned to calculate column densities for all masses which have significant counts.

In order to better identify sources of outgassing, it is planned to utilize the RMS to map the Shuttle surfaces. The IECM would be picked up out of the cargo bay by the RMS and maneuvered such that the MS and other instruments would be looking at certain critical surfaces. Again, it will be imperative to know where the MS is pointing at any given time.

These requirements for Shuttle attitude and altitude data as related to the IECM time clock have been requested and appear to be readily available.

It is expected that several weeks after each flight the necessary correlations will have been made and reduced data will be available. Identification of specific outgassing source materials may take longer (if at all possible) depending upon the complexity of mixtures and cracking

patterns. (Some discussion of this is given in Part II.) Comparison of data from flight to flight is expected to give an indication if the Shuttle and Shuttle bay can be expected to get cleaner with continued flights.

PART II

1.0 Introduction

The two major contamination effects which the MS will measure are: (1) a column density of molecules above the instrument which can interfere with observations (e.g., infrared adsorption) and (2) scattering of the effluents into the instruments which can degrade the optics.

The overall philosophy in conducting these IECM MS measurements would be to do them in such a fashion that they can be used to predict contamination effects under other operational conditions. The best method of implementing this philosophy is to conduct the measurements in a manner that they assess the validity of and update models which describe the phenomena of interest. The IECM MS will measure the return flux of both outgassed products and a special gas release. Simple models are available by which the column density can be determined from the return flux (details will be presented later). The column density determined from these measurements would then be compared to that predicted from models and the models updated/modified in an appropriate fashion. A computer code prepared by the Martin Marietta Corporation is now "in hand" and can calculate the column densities around the Shuttle under a wide variety of conditions. However, the column density of particles around the vehicle is a complex function of the magnitude of several sources such as: (1) surface outgassing/offgassing, (2) cabin/Spacelab leakage, (3) exhaust from thruster firings, and (4) water dumps (e.g., flash evaporator).

Even if the measured and predicted values were in good agreement, one could never be certain whether this resulted from an accurate model or a lucky set of circumstances. Therefore, to utilize the data obtained from the MS measurements and confidently predict future results, there should be an in situ measurement of the sources in order to verify the expressions describing their magnitude. In the following sections we will discuss both the MS measurements of backscattering/column density and also the type of data that should be obtained when measuring the Shuttle emissions.

2.0 Mass Spectrometer Measurements of Column Density

In Figure 8 we depict in a simplified fashion the interaction of an unperturbed atmospheric particle with an emitted particle which is part of the column density above the MS with its highly collimated aperture. The flux of particles reaching the aperture (area A) is approximately[4]

$$F \sim N_A(r) \quad N_o \left| \vec{V}_o - \vec{V}_A \right| \left(\frac{d\sigma}{dr} \right)_{s/c}^{\pi - \sigma} \frac{A}{r^2} (.1 \text{ str}) r^2 dr \tag{1}$$

where $N_A(r)$ is the density of the emitted particles around the body, N_o is the atmospheric density, $\left| \vec{V}_o - \vec{V}_A \right| \sim V_o$ is the velocity of the atmosphere relative to the emissions, A/r^2 is roughly the solid angle subtended by the MS seen by a distance r away, $(.1 \text{ str}) r^2 dr$ is the volume element above the MS, and $\left(\frac{d\sigma}{dr} \right)_{s/c}^{\pi - \sigma}$ is the probability that a particle will be scattered into angle $\pi - \sigma$ from the volume element. This equation assumes no additional scattering in the cloud above the MS which would tend to deflect the scattered particles away from the aperture. This limits the above equation to the regime where $\left(\int \sigma n(r)dr = \sigma N_R \leq 1 \right.$ (σ is the cross section assumed to be $\sim 3 \times 10^{-15}$ cm^2), or the column density (N_R) above the instrument $\sim 3 \times 10^{14}$/cm^2. For larger values of the column density, equation 1 would have to be modified to account for additional scatters; however, this could be done in a relatively straightforward manner. For the purposes of this paper we will assume that $N_R \leq 10^{14}$/cm^2 which is also consistent with the upper limits of N_R (i.e., $\sim 10^{12}$/cm^2) requested by the CRDG. The
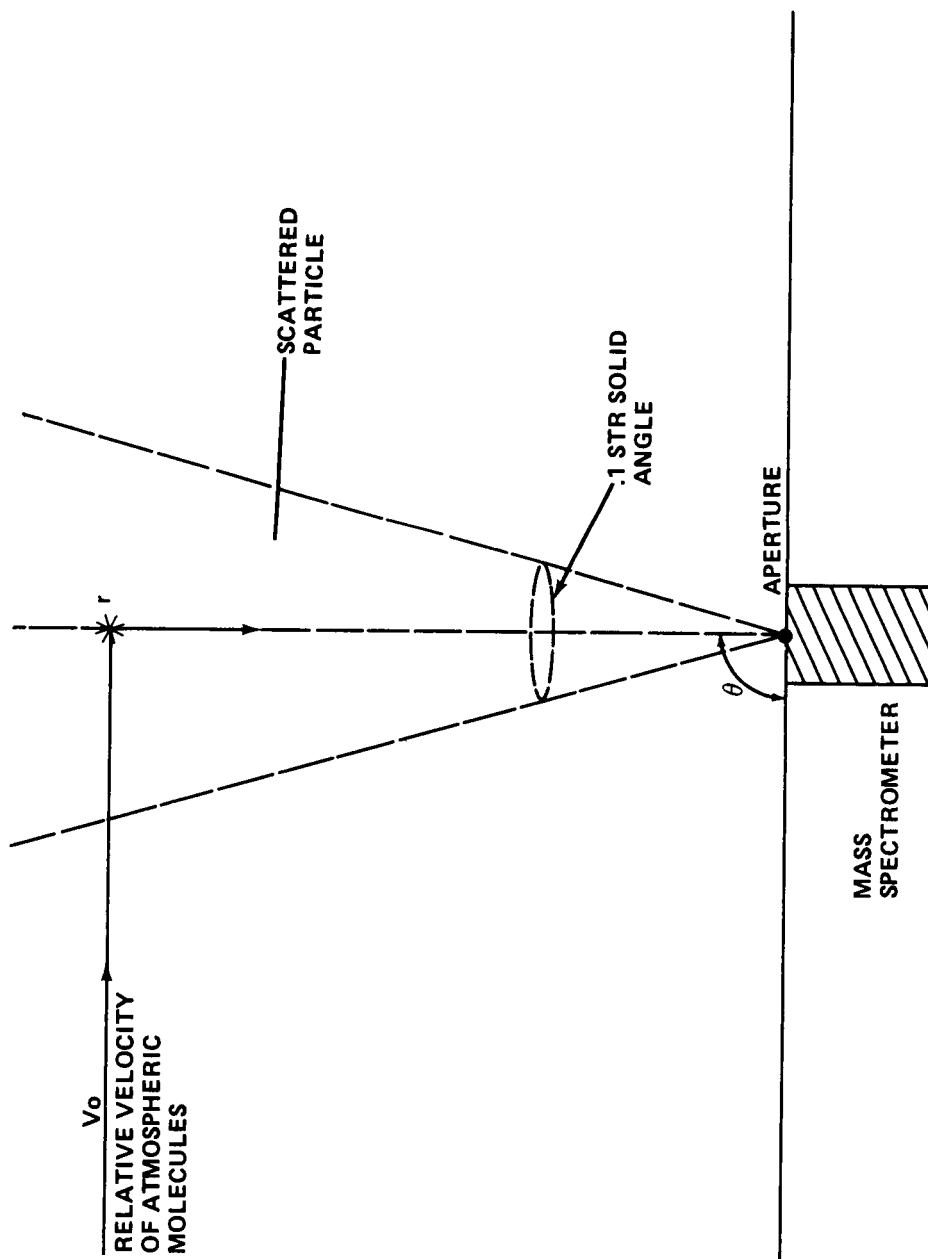
FIGURE 8. SIMPLIFIED PICTURE OF THE INTERACTION OF AN ATMOSPHERIC MOLECULE WITH A SPACECRAFT EMISSION AS SEEN BY THE MASS SPECTROMETER

function $\left(\dfrac{d\sigma}{dr}\right)^{\pi-\sigma}_{s/c}$ has been evaluated elsewhere for a collision which is isotropic in the center of mass (com) and equals $\dfrac{\sigma}{4\pi}\left(\sqrt{1-\beta^2\sin^2\sigma+2\beta\cos\sigma+}\right.$

$\left.\dfrac{\beta^2\cos^2\sigma}{\sqrt{1-\beta^2\sin^2\sigma}}\right)$ where $\beta=\dfrac{V_{com}}{V'}$, σ = cross section, and V_{com} = velocity

of the com, and V' is the velocity of the particle in the com after the collision.

Equation 1, therefore, becomes

$$\dfrac{F(\sigma)}{A}\sim N_R N_o V_o\,\sigma\left(\dfrac{1}{4\pi}\right)\left(\sqrt{1-\beta^2\sin^2\sigma}+2\beta\cos\sigma+\dfrac{\beta^2\cos^2\sigma}{\sqrt{1-\beta^2\sin^2\sigma}}\right)\quad(2)$$

Equation 2 needs some interpretation for the cases of $\beta\geq1$. An example of

this occurs in a partially inelastic collision where the particles scatter in

the com with a velocity less than V_{com}; in these instances $\sigma\leq90°$. For the

case of a completely inelastic collision $(\beta\to\infty)$, then both the particles

continue along a line defined by the direction of the incident particle or

$\sigma\sim0°$. In Figure 9 we have plotted the relative flux (i.e., $\dfrac{F(\sigma)}{AN_R N_o V_o\sigma\left(\frac{1}{4\pi}\right)}$)

for the case of an atmospheric atomic oxygen colliding with a relatively

stationary mass 22 particle. This was done for an elastic and an inelastic

collision where 90% of the energy in the com is dissipated. As can be seen

from this figure, the degree of inelasticity of the collision plays a dominant

role in determining the scattering pattern.

One of the principal difficulties in calculating the return scattered

fluxes (even if the column density is known) is inaccurate knowledge of

the parameters characterizing the interaction of the atmosphere (principally
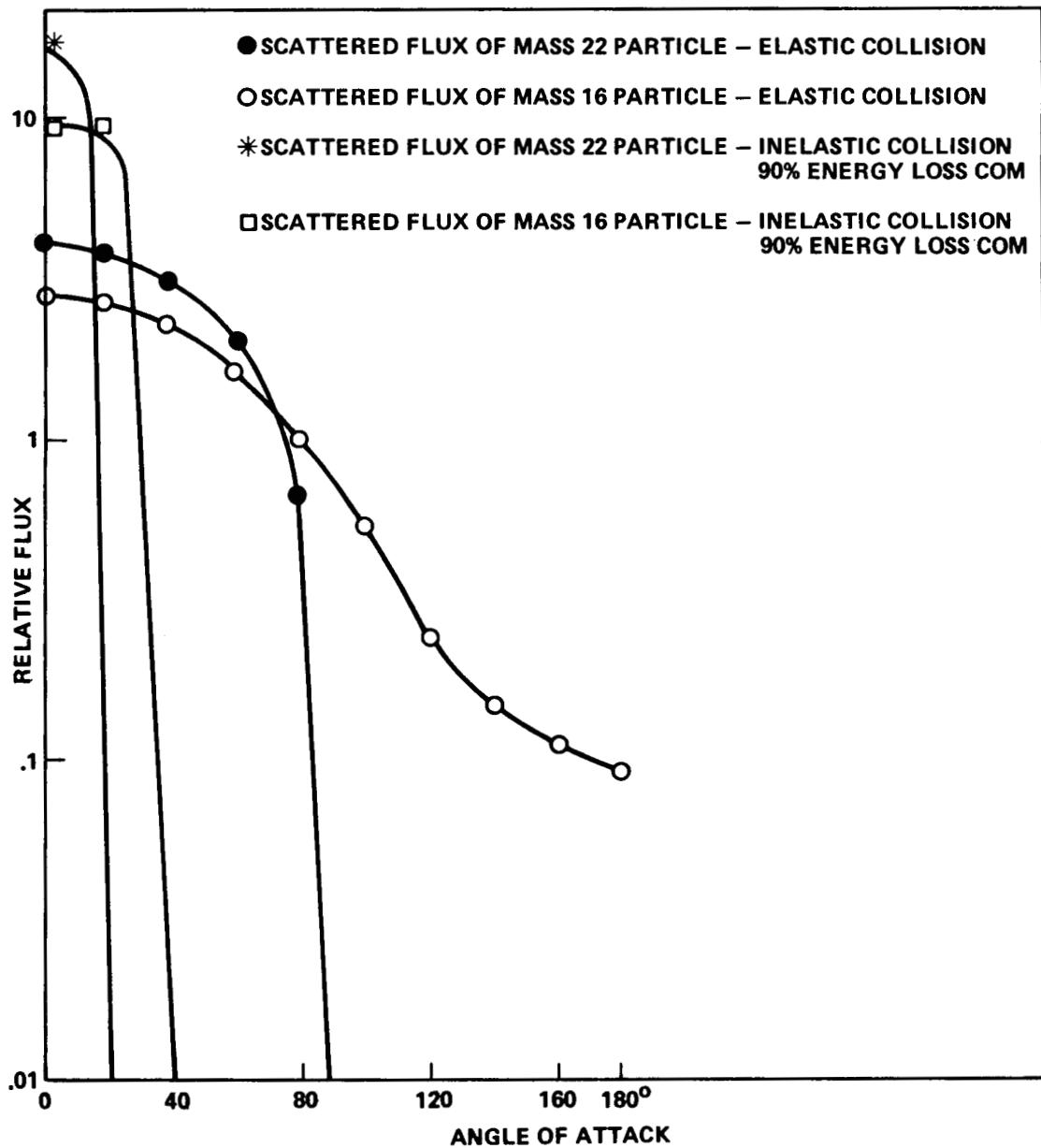
FIGURE 9. RELATIVE SCATTERED FLUX AS SEEN BY THE MASS SPECTROMETER. AN ATMOSPHERIC ATOMIC OXYGEN IS STRIKING A RELATIVELY STATIONARY (22 AMU) EMITTED ARTICLE AT 8km/sec. BOTH THE CASE OF AN ELASTIC AND INELASTIC COLLISION ARE PRESENTED.

atomic oxygen) with spacecraft emitted molecules at velocity differences of 8 km/sec (i.e., $V_o \sim 8$ km/sec). At this time one can only extrapolate from very fragmentary laboratory studies in defining parameters such as cross sections and degree of elasticity (i.e., parameter β). However, the controlled release of the Ne^{22}, D_2O gas cloud (mentioned previously) during the MS measurements can result in values being obtained for these parameters under actual in situ conditions. In fact, Figure 9 shows the type of data that might be expected from the release as both the MS and release system are slowly rotated through different angles of attack. The collision of the atomic oxygen and Ne^{22} should be basically elastic and the pattern for the scattered particles should be similar to that in Figure 9 for the elastic collision. On the other hand, one might expect the collision between the atomic oxygen and D_2O to excite various vibration/rotational levels and the patterns may be similar to those in Figure 9 for the inelastic collision.

Given the magnitude of the release $\sim 10^{19}$ molecules/sec and some assumptions of the geometry and velocity of the cloud, the anticipated N_R from the release is $\sim 10^{14}/cm^2$. This column density is sufficiently low that additional deflections in the cloud should not be significant. Using appropriate values for the MS aperture area, calibration constants and other constants, a curve fit of the in situ gas release data to equation 2 can give experimental values to parameters such as σ and degree of elasticity.

To define a column density of effluents above the Shuttle, the MS should be fixed in position and the Shuttle rotated in angle of attack so that a backscattered pattern similar to that of Figure 9 is obtained. Using the interaction parameters obtained from the gas release, a numerical value for the N_r can be obtained utilizing equation 2. For the case of H_2O the calculations should be fairly accurate. In the instance of other molecules (e.g., N_2 and O_2), one would have to assume that the interaction parameters are similar. This may not be the case, and it would be beneficial if additional gas release were conducted using a diatomic molecule instead of D_2O.

3.0 <u>Measurements of Shuttle Emission Characteristics</u>

As discussed before, to fully utilize the MS measurements and be able to confidently predict backscatter/column densities under a variety of in situ conditions, measurements must be made to validate the equations describing the in situ characteristics of Shuttle emissions. Fortunately, during part of the measurement program, a projected maneuver is to have the IECM picked up by the Remote Manipulator System and map the Shuttle emissions. This would allow an in situ characterizing of the sources. It is of interest to compare the magnitude of the various sources in order to establish their relative importance and priority for measurement purposes. The magnitude of cabin leakage has been specified at ~ 3 kgm/ day or $\sim .03$ gms/sec. Assuming an average outgassing rate of $\sim 10^{-10}$ gm/cm^2 sec for the non-metallic surfaces of Shuttle and total top

surface area of ~ 600 m^2, then the average outgassing rate of the upper

surfaces of Shuttle is $\sim 6 \times 10^{-4}$ gm/sec. The flash evaporator can eject

H_2O at a rate of up to ~ 90 kgm/day or ~ 1 gm/sec. While in orbit we

will assume that only the vernier thrusters will operate to control attitude,

and at a rate of a 40 msec thrust every minute there are ~ 2 gms of

material ejected/40 msec thrust or $\sim .03$ gms/sec.[5]

However, these very tentatively calculated rates have to be modified

by the following considerations:

a. Both the flash evaporator and the vernier thrusters generally

point down and away from the payload bay area, and the relative amount

of material effectly "seen" by an experiment can be considerably less than

that calculated depending upon how much impinges and is re-emitted by

the wings, etc.

b. The 3 kgm/day of cabin leakage could be an upper limit, and the

actual amount may be substantially less.

c. The desorption rate early in the mission is expected to be sub-

stantially greater than 10^{-10} gm/cm^2 sec.

It would, therefore, appear that at a first approximation all the sources

are equally important, and all should be measured. In particular, the

thermal dependence $\sim e^{+(T - 100^\circ C)/29^\circ C}$ of long-term outgassing and

both the thermal $e^{E/R(1/373 \cdot -1/T)}$ and temporal $e^{-t/18\ hrs}$ dependence

of the early desorption should be verified (E is the activation energy

~ 12 K cal/mole for H_2O and R = 2 K cal/mole $^\circ$K). The emission pattern of both the thrusters and flash evaporators should be checked, especially the rates for angles > 90° off nozzle axis since this portion of the emission can directly contribute to column densities above the bay.

Of the sources, it would appear that the species of emitted particles from the non-metallic surfaces would give the most complex (and least interpretable) MS spectra. This is due in part to the potential scavenging properties of atomic oxygen striking the surface. For example, at 250 km the environmental atomic oxygen will strike a surface orientated toward the ram direction at a flux rate of $\sim 10^{15}/cm^2$ sec. It is possible that the O will scavenge the atoms on the non-metallic surface as on metallic surfaces and be readmitted in molecular form (i.e., O_2, H_2O, CO).[6] In any event, assuming all the O is readmitted, the mass of these admissions is $\sim 3 \times 10^{-8}$ gms/cm^2 sec which is much greater than the surface emission rate mentioned earlier. Therefore, the impingement of atomic oxygen could well be the dominant effect of surface offgassing/outgassing, and the surface emissions should also be measured when exposed to the atomic oxygen flux.

To help assess the intrinsic capability of a mass spectrometer to detect the various species emitted from a surface, we have investigated the possibility of uniquely determining the species presently expected to be outgassed from the surface. Taking the early desorption from the teflon liner as typical we have the following rates:

$$H_2O \qquad \sim 5 \times 10^{13} \text{ molecules/cm}^2 \text{ sec}$$

$$N_2 \qquad \sim 2 \times 10^{13} \text{ molecules/cm}^2 \text{ sec}$$

$$CO_2 \qquad \sim 1 \times 10^{13} \text{ molecules/cm}^2 \text{ sec}$$

$$O_2 \qquad \sim 3 \times 10^{12} \text{ molecules/cm}^2 \text{ sec}$$

$$C_3H_{10}O_1Si_1 \qquad \sim 6 \times 10^{12} \text{ molecules/cm}^2 \text{ sec}$$

where the trimethyl silanol is assumed equivalent to the heavy molecule outgassing. Table I shows the relative fractionalization pattern as seen by the detector of the mass spectrometer based only on the above emission rates.[7] We can see by this characterizing example that, although some overlap is observed, the patterns of the individual molecules is sufficiently unique to unambiguously specify them. Therefore, it appears possible to uniquely determine the constituents outgassed from a surface for a "reasonable" grouping of species. We are also looking into the possibility of having a computerized search of several hundred compounds utilizing statistical techniques in order to analyze the mass spectrometer output in a more rigorous fashion.

TABLE I

Relative Intensities of Specific Masses Seen by a Mass Spectrometer after the Gas Molecules Have Been Fractionalized by the Ion Source

AMU Number	H_2O	N_2	Imput Molecules CO_2	O_2	$C_3H_{10}O_1Si_1$
12			13		
13			2		
14		20			
15					8
16	9		19	6	
17	211				
18	1000				
19	5				
20	3	2			
28		400	16		4
29					
32				160	
33				1	
34					
43					5
44			200		
45					29
47					15
59					15
61					3
75					120
76					7
77					4

In Summary

The IECM mass spectrometer is basically a highly collimated version of an instrument which has flown on the Atmospheric Explorer series and which was developed by the University of Michigan. The sensitivity of the instrument is $\sim 10^9 / cm^2$ sec for non-reactive gases. The principal measurements of the MS will be to measure directional backscattered rates and column densities due to Shuttle emissions. A controlled gas release of Ne^{22}, D_2O will allow a measurement of the interaction parameters (e.g., cross section and degree of elasticity) under in situ conditions. Utilizing the measured values of these parameters, one can then define the column density above the instrument. In addition, to be able to use this data and confidently predict the column densities under other in situ conditions, measurements must be made to verify the equations describing the strength of the sources of the Shuttle emissions.

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